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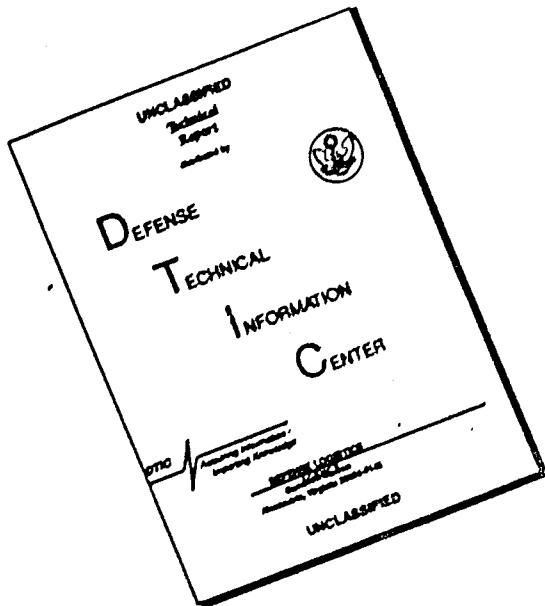
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FUNDAMENTAL RESEARCH IN APPLIED MATHEMATICS

ON THE NUMERICAL SOLUTION OF LINEAR AND NON-LINEAR
PARABOLIC EQUATIONS ON THE CRDVAC

by

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On the Numerical Solution of Linear and Non-Linear
Parabolic Equations on the Ordvac

by

David Young and Louis Burlich

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1. Introduction

Let us consider the problem of finding a function $u(x,y)$ which satisfies the parabolic partial differential equation

$$(1.1) \quad u_t = u_{xx} + f(x,t,u)$$

in $R: 0 < x < A, 0 < t < T$ and which satisfies the initial conditions

$$(1.2) \quad u(x,0) = g(x) \quad 0 < x < A$$

and the boundary conditions

$$(1.3) \quad \begin{cases} a_1(t)u_x(0,t) + \beta_1(t)u(0,t) = \phi(t) & 0 \leq t \\ a_2(t)u_x(A,t) + \beta_2(t)u(A,t) = \psi(t) & 0 \leq t. \end{cases}$$

The function $u(x,y)$ is required to be continuous and bounded in $R + S$, where S is the boundary of R , except that continuity of $u(x,y)$ is not required at a point of S where a jump discontinuity occurs in any of the other functions involved in (1.2) and (1.3). We assume that all functions are continuous and bounded in R .

An analytic solution for the above problem is available only under very special conditions. We shall not seek such solutions here. Moreover, we shall not even consider the very important questions of existence and uniqueness. Rather, we shall be concerned with the study of numerical procedures for solving certain difference equations which one obtains when one uses finite difference methods. Of course it is recognized that any solutions so obtained would be of no value in the event that no solution of the original problem existed or in the event that more than one solution existed. In certain cases existence

and uniqueness are available (See for instance [1] and [6]).

The numerical methods which we shall consider include the well-known Forward Difference method, the Crank-Nicolson method [4] and the DuFort-Frankel method [5]. With the Crank-Nicolson method one is usually required to solve at each step a system of simultaneous equations. This can be done effectively in many cases using the Successive Overrelaxation method of iteration [22]. Alternatively if the system is linear, or is replaced by a related linear system, one can use a non-iterative method, apparently first used for this type of problem by Bruce, Pesceman, Bachford, and Rice [2].

In section 2 we first derive finite difference representations of the boundary conditions including two well-known methods and one which we have not seen in the literature. We then derive several difference equations and obtain local error estimates using methods of numerical quadrature. Next, we consider the process known as "extrapolation to zero grid size", first used by L.F. Richardson [20]. Using this process one can, under favorable conditions, appreciably improve the accuracy of the finite difference methods. We indicate how results obtained using several different grid sizes can often be used to obtain a more accurate extrapolation formula than one would obtain using Richardson's formula wherein it is assumed that the error tends to zero like the square of the grid size.

In order to compare the various finite difference methods we prepared a comprehensive routine for Ordvac which is capable of solving a large class of problems by each method. Details of this program are given in section 4 and Appendix. The specific problems which we considered are discussed in section 3.

The program may be considered as a research tool to enable one to study the effectiveness of the various methods under different conditions. When used together with a more complete theoretical analysis than we have been able to carry out here, it is to be expected that new and significant results on finite difference methods should be obtained.

In section 5 the results obtained on the Orivac are analyzed and tentative conclusions are reached as to the order of convergence and the overall effectiveness of each of the methods. For the linear case our results indicate strongly that the use of the Crank-Nicolson method with the non-iterative procedure, is superior to any of the other methods. In the non-linear case however, one loses accuracy with this method if one modifies the difference equation in an attempt to avoid all iterations. Further work appears to be indicated in order to preserve the accuracy of the difference equation without requiring too many iterations. We suggest one possible scheme for doing this, but we have not yet tried it out on the machine.

For the Forward Difference method and for the Crank-Nicolson method, used with the iterative process, we found that the accuracy could usually be improved considerably by the use of the proper extrapolation to zero grid size. Such extrapolation was more difficult to carry out for the Crank-Nicolson method, used without iterations.

As expected the use of the proposed method for representing the boundary conditions appeared to be more accurate than either of the other two considered.

Although this study is far from complete, it was felt that the work which has been done to date should be reported now, especially since no further work can be done during the next academic year. The work may be regarded

4

as a natural extension of research which was begun by the Interior Ballistics Laboratory, Aberdeen Proving Ground. One of the objects was to determine the order of convergence of the Forward Difference method. Extensive calculations were carried out on the Bell Relay Computer, as described in [6], and on the Eniac. The latter calculations have not previously been reported. We shall study them in section 5 along with the Ordvac results.

In addition to acknowledging the sponsorship of the Office of Ordnance Research, U.S. Army, we should also like to express our appreciation for the encouragement and assistance furnished by the Interior Ballistic Laboratory at the Aberdeen Proving Ground. Discussions with Dr. W.C. Taylor of the Interior Ballistic Laboratory and with Dr. B.L. Hicks, formerly of that laboratory, were of great value. We are also pleased to acknowledge the assistance of Dr. R.M. Conlan, Miss J.M. Wood, Mr. B.I.C. Koo, and Mr. S. Soscia who worked at various times on the programming of the problem for Ordvac.

2. Difference Equations

Let h and k be positive numbers such that A/h is an integer, which we denote by N , and let $L_{h,k}$ denote the set of points (x,t) such that x/h and t/k are integers. Let $R_{h,k}$ and $S_{h,k}$ denote respectively the set of points of $L_{h,k}$ belonging to R and to S , (See Figure 1). We replace the problem of the previous section by that of finding a function $u(x,t)$ defined on $R_{h,k} \cup S_{h,k}$, satisfying a certain difference equation on $R_{h,k}$ and satisfying on $S_{h,k}$ certain other conditions derived from (1.2) and (1.3).

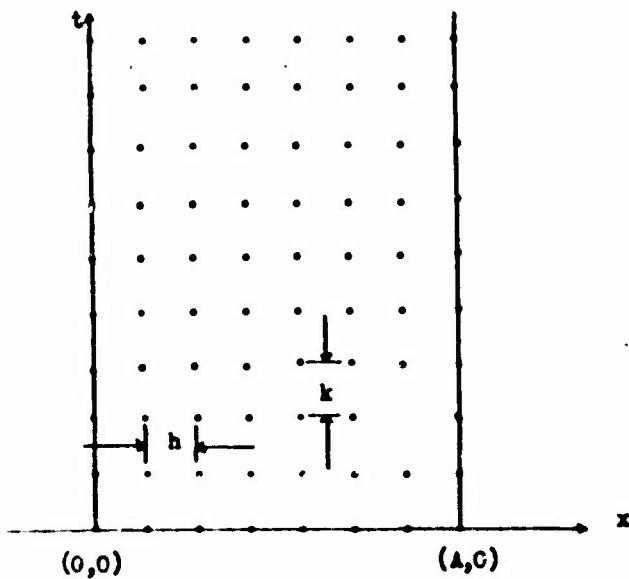


Figure 1

In this section we derive finite difference equations, which are obtained from the differential equation and from the boundary conditions, and seek to estimate the accuracy. Our methods are by no means rigorous. Indeed they are merely formal methods utilizing Taylor series expansions whenever convenient. Nevertheless, it is felt that these methods will give some basis for making comparisons of the accuracies of the various finite difference methods, at least

for some cases. We will later test the comparisons thus obtained against numerical results obtained for typical problems on the Ordvac.

For discussion of finite difference analogues of problems involving the infinite region $\rightarrow \infty$ the reader is referred to papers by Courant, Friedrichs and Lewy [3] and by Fitts John [10].

In addition to deriving the difference equations we will also describe here the associated numerical procedures. In order that we may be able to give a complete description of these procedures it is convenient to first consider the treatment of the boundary conditions.

2.1 Boundary conditions. Although our discussion could be extended to cover more general situations, we shall consider only the following two types of boundary conditions

$$(2.1.1) \quad \begin{cases} (a) \quad u(0,t) = \phi(t), & (t \geq 0) \\ (b) \quad u(A,t) = \psi(t), & (t \geq 0), \end{cases}$$

and

$$(2.1.2) \quad \begin{cases} (a) \quad u_x(0,t) = -H(u_g - u(0,t)), & (t > 0) \\ (b) \quad u_x(A,t) = 0 & (t > 0). \end{cases}$$

Here H and u_g are constants.

We shall at times refer to the boundary conditions represented by (2.1.1) and (2.1.2) as B V and N D conditions, respectively.

We first note that the initial conditions (1.2) are easily represented by

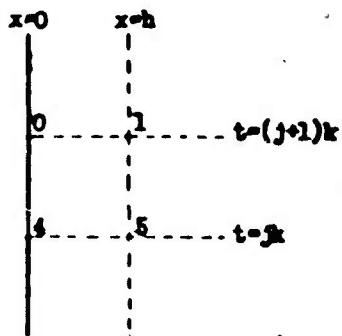
$$(2.1.3) \quad u_{i,0} = g_i \quad 1 \leq i \leq M-1.$$

Here and subsequently we let $u_{i,j} = u(ih, jk)$, $g_i = g(ix)$, etc., where i and j are integers. Moreover, the B V conditions (2.1.1) can be replaced by

$$(2.1.4) \quad \begin{cases} u_{0,j} = \phi_j, & (0 \leq j) \\ u_{M,j} = \psi_j, & (0 \leq j). \end{cases}$$

However, with the ND condition (2.1.2a) we shall consider several alternative procedures. A number of these are considered by Price and Slack [9]. We shall discuss two of these together with one which may very well be known also, although we have not seen it in the literature.

In order to simplify our notation we shall consider a configuration of four points near the line $x = 0$, as shown in Figure 2. We denote by u_i , t_i , x_i , f_i the values of the respective variables at the point numbered i , ($i = 0, 1, 4, 5$). We seek relations between u_0 and one or more of the other u_i . It



Typical Boundary Configuration - Left Hand Boundary

Figure 2

is assumed that u_4 and u_5 have already been obtained by previous calculations.

Perhaps the most obvious method is to replace $u_x(0,t)$ by $(u_1 - u_0)h^{-1}$ in (2.1.2a) obtaining

$$(2.1.5) \quad u_0 \approx \frac{u_1 + h u_x}{1 + h u_x} .$$

Formula (2.1.5) defines a procedure for representing (2.1.2a) which we shall refer to as Option I.

To study the accuracy of (2.1.5) we expand $u(x,t)$ in a Taylor series about the point (x_0, t_0) obtaining

$$u_1 = u_0 + h u_x + \frac{h^2}{2} u_{xx} + \dots$$

Using (2.1.2a) we obtain

$$(2.1.6) \quad u_0 = \frac{u_1 - h u_x}{1 + h u_x} = - \frac{h^2}{2(1+h u_x)} u_{xx} + \dots$$

We note that the leading term of the local error, given by the right member of (2.1.6) is $O(h^2)$. We shall not try to estimate here the effect of local errors on the accuracy of the solution of the difference equation as a solution of the

differential equation. Instead we shall attempt to infer this from the results of Ordvac computations.

If one makes use of the differential equation at the point (x_4, t_4) , one can obtain more accurate formulas. Thus, using a Taylor series expansion about (x_4, t_4) we have

$$u_0 = u_4 + hu_t + \frac{1}{2}h^2u_{tt} + \dots$$

$$u_5 = u_4 + hu_x + \frac{1}{2}h^2u_{xx} + \frac{1}{6}h^3u_{xxx} + \dots$$

Here the derivatives are evaluated at (x_4, t_4) . Using (1.1) and the relation $u_x = -H(u_g - u_4)$ we obtain

$$(2.1.7) \quad u_0 \approx u_4(1-2r) + 2ru_5 + 2rhH(u_g - u_4) + kf_4$$

where the leading terms of the difference between the right and the left members of (2.1.7), that is, the right member minus the left member, are

$$(2.1.8) \quad -\frac{1}{3}h^3u_{xxx} + \frac{k^2}{2}u_{tt}.$$

Here and subsequently we let

$$(2.1.9) \quad r = \frac{k}{h^2}.$$

Price and Slick [19] show that this formula introduces instability for $r > \frac{1}{2}$, in contrast to (2.1.5) which is stable for all r . Thus assuming $k = rh^2$, where r is a constant not greater than $\frac{1}{2}$, we obtain from (2.1.8)

$$(2.1.10) \quad -\frac{rh^3}{3}u_{xxx} + \frac{rh^4}{2}u_{tt}.$$

Thus the leading term of the local error is $O(h^3)$ as compared with $O(h^2)$ with Option I. Unfortunately, however, as we shall see later, the limitation which must be imposed on k is very severe.

We shall refer to (2.1.7) as Option II.

We now seek a formula which is as accurate as Option II and which is, at the same time, stable for all r . With this aim we expand $u(x,t)$ in a Taylor series about the point (x_0, t_0) obtaining

$$u_1 = u_0 + hu_x + \frac{1}{2}h^2u_{xx} + \frac{1}{6}h^3u_{xxx} + \dots$$

$$u_4 = u_0 - ku_t + \frac{1}{2}k^2u_{tt} - \frac{1}{6}k^3u_{ttt} + \dots$$

Using (2.1.2a) and (1.1) we have

$$(2.1.11) \quad u_0 \approx \frac{u_1 + hHu_g + \frac{1}{2r}u_4 + \frac{1}{2}h^2f_0}{1 + hH + \frac{1}{2r}}$$

where the leading term of the difference between the right and left members of (2.1.11) is

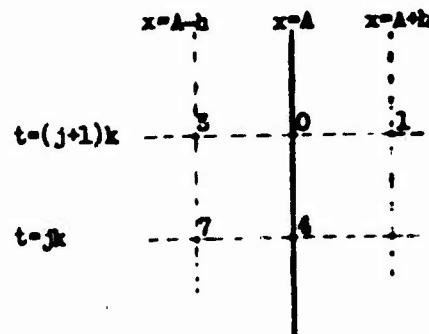
$$(2.1.12) \quad \frac{-\frac{1}{4}h^2ku_{tt} - \frac{1}{6}h^3u_{xxx}}{1 + hH + \frac{1}{2r}}.$$

Evidently the leading term of the local error for (2.1.11), which we shall call Option III, is $O(h^2k + h^3)$. Moreover, since all coefficients in (2.1.11) are positive, the formula is stable for all r .

In some cases it is convenient to replace f_0 by f_4 in (2.1.11), obtaining

$$(2.1.13) \quad u_0 \approx \frac{u_1 + hHu_g + \frac{1}{2r}u_4 + \frac{1}{2}h^2f_4}{1 + hH + \frac{1}{2r}},$$

where the numerator in (2.1.12) is changed by a term whose absolute value is $\frac{1}{2}h^2kf_t^*$, where $f_t^* = f_t + f_uu_t$. Since this term is $O(h^2k)$, the order of the local accuracy of (2.1.13) is the same as that of (2.1.11). We will refer to (2.1.13) as Option III'.



Typical Boundary Configuration - Right hand Boundary

Figure 3

We now consider the treatment of (2.1.2b). For the simplest representation we replace u_x by $(u_0 - u_3)h^{-1}$ obtaining

$$(2.1.14) \quad u_0 \approx u_3.$$

It is easily seen that the leading term of the difference between the right and left members of (2.1.14) is

$$-\frac{h^2}{2} u_{xx}$$

so that (2.1.14) has the same accuracy as Option I. Actually, of course, (2.1.14) is a special case of (2.1.5) where $H = 0$.

Formula (2.1.14) represents the only method which we used for treating (2.1.2b). Perhaps a better procedure would have been to consider (x_0, y_0) as an interior point and to use

$$(2.1.15) \quad u_1 \approx u_3.$$

Here, the leading term of the error is

$$\frac{h^3}{3} u_{xxx},$$

which is $O(h^3)$.

If one does not wish to use the point (x_1, t_1) , which is outside the region, one may obtain a formula of the same order of accuracy by using the point (x_4, t_4) instead. The formula may be obtained immediately from (2.1.11) by letting $\Xi = 0$.

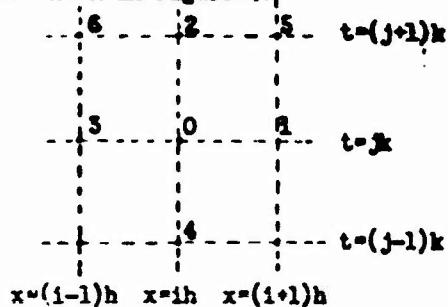
We get

$$(2.1.16) \quad u_0 \approx \frac{u_1 + \frac{1}{2r} u_4 + \frac{1}{2} h^2 f_0}{1 + \frac{1}{2r}} .$$

The leading term of the error is $O(h^3)$. As before the accuracy would be preserved if we replaced f_0 by f_4 in (2.1.16), obtaining

$$(2.1.17) \quad u_0 \approx \frac{u_1 + \frac{1}{2r} u_4 + \frac{1}{2} h^2 f_4}{1 + \frac{1}{2r}} .$$

2.2 Forward difference method. For the derivation of this and other difference equations it will be convenient to consider a typical configuration of points such as shown in Figure 4.



Typical Configuration - Interior Points

Figure 4

We assume here that $1 \leq i \leq N-1$, but that j may equal zero in which case the point (x_j, t_j) would lie outside of the region.

Probably the simplest difference equation is obtained by replacing u_t by $(u_2 - u_0) k^{-1}$ and by replacing u_{xx} by $(u_1 + u_3 - 2u_0) h^{-2}$. These are familiar finite difference representations of the respective derivatives. However, for this method and for the others given below we shall present a derivation based on methods of numerical quadrature. Although the actual finite difference formulas come out the same, nevertheless it seems simpler to obtain the error estimates by the method which we use.

By (1.1) and the rectangle rule for integration we have

$$(2.2.1) \quad u_2 - u_0 = \int_{t_0}^{t_0+k} u_t dt = \int_{t_0}^{t_0+k} (u_{xx} + f) dt = k(u_{xx} + f) + \frac{k^2}{2}(u_{xxt} + f'_t),$$

where $f'_t = f_t + f_{tt} u_t$. Using Taylor's series we also obtain

$$(2.2.2) \quad u_{xx} = (u_1 + u_3 - 2u_0)h^{-2} - \frac{1}{12}h^2 u_{xxxx} + \dots$$

Substituting in the previous equation we get

$$(2.2.3) \quad u_2 = (1-2r)u_0 + r(u_1 + u_3) + kf_0$$

where the leading term of the difference between the right and left members of (2.2.3) is

$$(2.2.4) \quad k \left\{ \left(\frac{k}{2} - \frac{h^2}{12} \right) u_{xxxx} \right\}.$$

Since the number of time steps needed to reach a given value of t is proportional to k^{-1} it seems reasonable to take

$$(2.2.5) \quad \left(\frac{k}{2} - \frac{h^2}{12} \right) u_{xxxx}$$

as a measure of the local error. It is well known, (See for instance [18]) that k must satisfy the condition

$$(2.2.6) \quad k \leq \frac{1}{3}h^2$$

in order for the numerical procedure to be stable. Thus the local error for the Forward Difference method is $O(h^2)$.

Of course, such an analysis does not, by any means, indicate that the accuracy in the large is of second order. The question of the order of convergence in the large has been studied for a special class of problems by Juncosa and Young [12]. For an analysis of the situation in the large for the case where $u(x,t)$ is assumed to possess certain partial derivatives in R+S, see Milne [17].

For B V problems with f, ϕ, f' vanishing, the convergence of the sequence of solutions of the Forward Difference method to the exact solution of the differential equation has been proved by Lauter [16] for $r \leq 1/4$, under the assumption that $g(x)$ is piecewise continuous, that is, continuous except for a finite number of finite jumps, and that $g(x)$ has a one sided first derivative everywhere. Hildebrand [9] proved convergence for $0 < r \leq \frac{1}{3}$ under the assumption that $g(x)$

is piecewise continuous and has bounded variation. More severe restrictions were imposed on $g(x)$ for the case $r = \frac{1}{2}$. Juncosa and Young [11] proved convergence for $r \leq \frac{1}{2}$ under the assumption that $g(x)$ is piecewise continuous.

The numerical computational procedure is extremely simple. Since one knows $u_{1,0}, 0 \leq i \leq M$, one can compute $u_{1,1}, 1 \leq i \leq M-1$ using (2.2.3) which for a general point becomes

$$(2.2.7) \quad u_{1,j+1} = (1-2r)u_{1,j} + r(u_{1+1,j} + u_{1-1,j}) + kf_1.$$

For B V problems $u_{0,1}$ and $u_{M,1}$ are given and we can proceed at once to the next row. For N D problems we can compute $u_{0,1}$ directly from either (2.1.5) or (2.1.7) or (2.1.13) and we can use (2.1.14), (2.1.15) or (2.1.17) to find $u_{M,1}$. Having thus determined all values of $u_{1,1}$ we proceed to compute values of $u_{1,2}$ then $u_{1,3}$ etc.

Were it not for the condition (2.2.6) on the size of k , the Forward Difference method would be ideal for use on computing machines. Unfortunately, when one attempts to improve the accuracy by reducing h , say by a factor of 2, then the number of time steps is increased by a factor of 4, making the total work increase by a factor of 8. More generally, one can assert that the work increases with the third power of h^{-1} , or equivalently, as the third power of M .

2.3 Crank-Nicolson method. If, instead of using the rectangle rule of integration as in the case of the forward difference method, we use the trapezoidal rule, we obtain

$$(2.3.1) \quad u_2 - u_0 = \int_{t_0}^{t_0+k} u_t dt = \int_{t_0}^{t_0+k} (u_{xx} + f) dt \\ = \frac{k}{2} [(u_{xx})_0 + (u_{xx})_2 + f_0 + f_2] - \frac{k^3}{12} (u_{xxxx} + f_{tt}) + \dots$$

Using Taylor's series we have

$$(u_{xx})_0 = h^{-2}(u_1 + u_3 - 2u_0) - \frac{h^2}{12} u_{xxxx} + \dots$$

$$(u_{xx})_2 = h^{-2}(u_5 + u_6 - 2u_2) - \frac{h^2}{12} u_{xxxx} + \dots$$

Substituting in (2.3.1) we get

$$u_2 = u_0 + \frac{k}{2h^2} [u_1 + u_3 + u_5 + u_6 - 2u_0 - 2u_2] + \frac{k}{2}[f_0 + f_2] - \frac{kh^2}{12} u_{xxxx} - \frac{k^3}{12} (u_{xxxx} + f_{tt}).$$

Solving for u_2 we have

$$(2.3.2) \quad u_2 = \frac{1-r}{1+r} u_0 + \frac{r}{2(1+r)} [u_1 + u_3 + u_5 + u_6] + \frac{k}{2(1+r)} [f_0 + f_2]$$

where we have neglected the remainder whose leading terms are

$$(2.3.3) \quad \frac{k}{1+r} \left\{ -\frac{h^2}{12} u_{xxxx} - \frac{k^2}{12} (u_{xxxx} + f_{tt}) \right\}.$$

We note that the expression in the braces is $O(h^2)$ as long as $k = O(h)$. Juncosa and Young [13] showed that under certain conditions the error in the large is $O(h^2)$ provided $k = O(h/\log h)$. It is not known, however, whether this result can be extended to include cases where $k = O(h)$.

It is sometimes convenient to replace f_2 by f_0 in (2.3.2). The additional error which is introduced is proportional to k^2 and hence the expression in braces occurring in (2.3.3) is increased by a term proportional to k . Thus if k tends to zero like h , the expression in the braces would be $O(h)$ instead of $O(h^2)$.

Another modification of (2.3.2) is obtained by replacing the term $\frac{1}{2}[f_0 + f_2]$ by $f(x_0, \frac{1}{2}(t_0+t_2), \frac{1}{2}(u_0+u_2))$. This change was made in the program prepared for the Ordvac. For simplicity, we assume here that $f(x, t, u)$ is a function of

u alone. Expanding in a Taylor series about the point (x, \bar{t}) , where $\bar{t} = \frac{1}{2}(t_0 + t_2)$

we have $u_2 = \bar{u} + \frac{1}{2}ku_t + \frac{1}{8}k^2u_{tt} + \dots$

$$u_0 = \bar{u} - \frac{1}{2}ku_t + \frac{1}{8}k^2u_{tt} + \dots$$

$$f_2 = \bar{f} + \frac{1}{2}kf_t + \frac{1}{8}k^2f_{tt} + \dots$$

$$f_0 = \bar{f} - \frac{1}{2}kf_t + \frac{1}{8}k^2f_{tt} + \dots$$

where $\bar{f} = f(\bar{u}), \bar{u} = u(x, \bar{t})$. It is evident that $\frac{1}{2}(f_0 + f_2) = \bar{f} + \frac{1}{8}k^2f_{tt} + \dots$

and $\frac{1}{2}(u_0 + u_2) = \bar{u} + \frac{1}{8}k^2u_{tt} + \dots$

Therefore $f(\frac{1}{2}(u_0 + u_2)) = \bar{f} + \frac{1}{8}k^2u_{tt} + \dots$

and $f_0 + f_2 - f(\frac{1}{2}(u_0 + u_2)) = \frac{1}{8}k^2f_{tt} - \frac{1}{8}k^2u_{tt} + \dots = O(k^2)$.

By (2.3.2) and (2.3.3) it is evident that the order of accuracy has not been changed.

For a general point (2.3.2) may be written

$$(2.3.4) \quad u_{i,j+1} = \frac{1-r}{1+r}u_{i,j} + \frac{r}{2(1+r)}[u_{i+1,j} + u_{i-1,j} + u_{i+1,j+1} + u_{i-1,j+1}]$$

~~$+ \frac{r}{2(1+r)}[f_{i,j} + f_{i,j+1}]$~~

Two alternative numerical procedures are available for using the Crank-Nicolson method. The first is an iterative method wherein, given all values of $u_{i,j}$, $0 \leq i \leq M$, one chooses a first approximation $u_{i,j+1}^{(0)}$, $0 \leq i \leq M$ and proceeds to iterate using the formula

$$(2.3.5) \quad u_{i,j+1}^{(n)} = \omega \left\{ \frac{1-r}{1+r}u_{i,j} + \frac{r}{2(1+r)}[u_{i+1,j} + u_{i-1,j} + u_{i+1,j+1}^{(n-1)} + u_{i-1,j+1}^{(n-1)}] \right. \\ \left. + \frac{r}{2(1+r)}[f_{i,j} + f_{i,j+1}^{(n)}] \right\} - (\omega-1)u_{i,j}^{(n)}, \quad i=1, \dots, M-1.$$

Here the parameter ω known as the relaxation factor, is chosen in the range $1 \leq \omega < 2$ to accelerate the convergence. At the end of each iteration one obtains $u_{0,j+1}^{(n)}$ by solving (2.1.5), (2.1.7), (2.1.11), or (2.1.13) for $u_{0,j+1}^{(n)}$ using the latest values of $u_{i,j+1}^{(n)}$ when appropriate. Similarly $u_{M,j+1}^{(n)}$ is obtained.

The iterative process is repeated until

$$(2.3.6) \quad \max_{0 \leq i \leq M} |u_{i,j+1}^{(n)} - u_{i,j+1}^{(n-1)}| < \epsilon$$

where ϵ is a preassigned tolerance. When the iterative process has converged, one proceeds to determine the values in the next row in the same way.

The choice of the relaxation factor ω_b , which will yield the fastest convergence can easily be computed for linear BV problems. It is shown in [22] that

$$(2.3.7) \quad \omega_b = 1 + \left[\frac{\mu}{1 + \sqrt{1 - \mu^2}} \right]^2$$

where μ is the maximum eigenvalue of the $(M-I)x(M-I)$ matrix

$$\begin{pmatrix} 0 & \beta & 0 & \dots & 0 \\ \beta & 0 & \beta & \dots & 0 \\ 0 & \beta & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & \beta \end{pmatrix}$$

where $\beta = \frac{r}{2(1+r)}$. It is easy to show that

$$(2.3.8) \quad \mu = \frac{r}{1+r} \cos \frac{\pi}{M}.$$

Let us now assume that $k = O(h)$ and that, as a result, r is proportional to M . Since for large M we have $1-\mu \approx \frac{1}{M}$, we can show, as in [22], section 4, that the rate of convergence of (2.3.5) varies as $M^{-\frac{1}{2}}$; hence the number of iterations increases as $M^{\frac{1}{2}}$. Since the number of points on each row increases with M , it follows that the work per row is proportional to $M^{3/2}$. Moreover, since the number of time steps increases as M , (instead of M^2 as with the Forward Difference method) we conclude that the total time increases as $M^{5/2}$ with the Crank-Nicolson method compared with M^3 for the Forward Difference method. Thus the Crank-Nicolson method would appear to be superior to the Forward Difference method, at least for large M .

The advantage of the Crank-Nicolson method can be increased still further by using a non-iterative procedure. The effectiveness of this procedure depends on the fact that for a linear system involving a Jacobi matrix, i.e., a matrix whose only non-zero elements occupy the main diagonal and the two diagonals adjacent to the main diagonal, the solution can be obtained very easily. This fact was observed by L.H. Thomas in unpublished notes [2] and was applied to parabolic equations by Bruce, Peaceman, Rachford and Rice [2]. Thus following their discussion, let us suppose we have the system

$$(2.3.9) \quad \begin{cases} B_1x_1 + C_1x_2 = d_1 \\ A_1x_{1-1} + B_1x_1 + C_1x_{1+1} = d_1 \\ A_{M-1}x_{M-1} + B_Mx_M = d_M \end{cases} \quad 2 \leq i \leq M-1$$

If one carries out the familiar Gauss elimination procedure, eliminating the elements below the main diagonal of the matrix, and then uses the method of back substitution, one obtains

$$(2.3.10a) \quad \begin{cases} x_M = q_M \\ x_i = q_i - b_i x_{i+1} \end{cases} \quad 1 \leq i \leq M-1$$

where

$$(2.3.10b) \quad \begin{cases} q_1 = d_1/B_1 \\ q_i = \frac{d_i - A_1q_{i-1}}{B_i - A_i b_{i-1}} \end{cases}$$

and

$$(2.3.10c) \quad \begin{cases} b_0 = 0 \\ b_i = \frac{C_i}{B_i - A_i b_{i-1}} \end{cases} \quad 1 \leq i \leq M-1.$$

The stability of the computation procedure has been investigated by Thomas in [2].

No more than about 3 or 4 times as much work per row would appear to be required with this method as with the Forward Difference method. Thus, if we assume $k = O(h)$, then the amount of work required increases as M^2 instead of $M^{5/2}$ with the iterative procedure and M^3 with the Forward Difference method.

Unfortunately, when (1.1) is non-linear it is not always easy to obtain linear equations and still retain the desired accuracy. Nor, if we use (2.3.2), do we find that the unknown value of $u_{i,j+1}$ is involved, in general, in a non-linear manner in the evaluation of the function $f(x,t,u)$. On the

other hand, if one replaces $u_{i,j+1}$ by $u_{i,j}$, one obtains a less accurate formula, as discussed above. To get around this difficulty in an analogous situation, Bruce, Peaceman, Rachford, and Rice [2] used an iterative procedure together with the non-iterative method for solving the linear equations. Although this procedure might appear to defeat the original purpose of avoiding all iterations, it is reported that convergence is obtained after a very few iterations.

It might not be too unreasonable to preassign a fixed number of iterations, independent of h and k , to be carried out at each time step. Thus, the Heun method for solving ordinary differential equations is the same as the modified Euler method (see for instance, Milne [17]) except that one performs only one iteration. The local error for the Heun method is somewhat larger than, but of the same order of magnitude as the modified Euler method.

Another possible solution to this difficulty would be to use a difference equation involving more points. However, care must be taken to avoid formulas which might lead to unstable procedures, and also to avoid obtaining a matrix which was not a Jacobi matrix.

2.4 DuFort-Frankel method. In [5] DuFort and Frankel obtained a difference equation which is stable for all values of r and which, at the same time, yields explicit formulas for values of u in the new row in terms of values on previous rows. We may derive the formula by use of numerical quadrature as follows.

$$(2.4.1) \quad u_2 - u_4 = \int_{t_4}^{t_2} u_t dt = \int_{t_4}^{t_2} (u_{xx} + f) dt \\ = 2k [u_{xx} + f_0] + \frac{1}{3} k^3 [u_{xxt} + f_t^0] + \dots .$$

Using Taylor's series, as before, we get

$$(2.4.2) \quad u_2 = u_4 + 2k[(u_1 + u_3 - 2u_0)h^{-2} + f_0] + \left\{ -2k \frac{h^2}{12} u_{xxxx} \right. \\ \left. + \frac{k^3}{3} (u_{xxt} + f_t^*) \right\} + \dots$$

If we were to neglect the expression in the braces and all higher order terms in (2.4.2) we would obtain Richardson's method [20], which is unstable for all values of r and is thus unsuited for numerical calculations unless very special precautions are taken [15]. Nevertheless, at this point we remark that the local error for Richardson's method is

$$(2.4.3) \quad k \left\{ -\frac{h^2}{6} u_{xxxx} + \frac{k^2}{3} (u_{xxt} + f_t^*) \right\}.$$

In order to obtain a stable method, DuFort and Frankel replace u_0 by $\frac{1}{2}(u_4 + u_2)$ in (2.4.2) and obtain, after solving for u_2 ,

$$(2.4.4) \quad u_2 = \frac{1-2r}{1+2r} u_4 + \frac{2r}{1+2r} (u_1 + u_3) + \frac{2k}{1+2r} f_0 \\ + \frac{k}{1+2r} \left\{ -\frac{h^2}{6} u_{xxxx} + \frac{k^2}{3} (u_{xxt} + f_t^*) - \frac{2k^2}{h^2} u_{tt} \right\} + \dots$$

Now if $k = O(h^2)$, it is evident that the expression in the braces is $O(h^2)$. On the other hand, if $k = O(h)$, then the expression inside the braces need not even tend to zero with h . Consequently, although stability is assured for all h and k , for convergence the ratio k/h must tend to zero with h , (see [5]).

Neglecting remainder terms we have for a general point

$$(2.4.5) \quad u_{i,j+1} = \frac{1-2r}{1+2r} u_{i,j-1} + \frac{2r}{1+2r} (u_{i+1,j} + u_{i-1,j}) + \frac{2k}{1+2r} f_{i,j}.$$

Evidently, to compute $u_{i,j+1}$, one needs the values of u on the j -th and $(j-1)$ st rows. At the beginning one has only the values for $j = 0$. To obtain the values

of u for $j = 1$ another procedure must be used. This point is discussed further in Section 4.

The convergence of the DuFort-Frankel method for a certain class of problems has been given by Juncosa [14].

2.5. Extrapolation to zero grid size. For the process known as extrapolation to zero grid size, proposed by L. F. Richardson [20], one assumes that the error $e_M(x,t) = u_M(x,t) - u(x,t)$ is proportional to h^6 . Here $u(x,t)$ is the exact solution of the differential equation and $u_M(x,t)$ is the solution of the difference equation with $h = A/M$. Usually certain restrictions are assumed for k . Even though $e_M(x,t)$ might vanish like M^{-6} , as is indeed true for certain cases as shown in [12], [13], nevertheless it does not necessarily follow that $e_M(x,t)$ is exactly proportional to M^{-6} . This can be easily seen by considering the case where $e_M(x,t) = M^{-6} \sin M$.

If $e_M(x,t)$ were directly proportional to M^{-6} , one could determine $u(x,t)$ in terms of $u_M(x,t)$ and $u_{2M}(x,t)$. Indeed we would have

$$(2.5.1) \quad u(x,t) = u_{2M}(x,t) + \frac{1}{2^{k-1}} [u_{2M}(x,y) - u_M(x,y)].$$

If one solves the difference equation for three different mesh sizes, obtaining $u_M(x,y)$, $u_{2M}(x,y)$, and $u_{4M}(x,y)$ we can perform a simple test for the assumption that $e_M(x,y)$ is proportional to M^{-6} . Indeed, if the assumption were valid, we would have

$$(2.5.2) \quad \frac{u_4(x,y)}{u_{2M}(x,y)} = 2^6.$$

By computing the ratio, ρ , appearing in (2.5.2) one can determine the proper extrapolation to zero grid size, provided such exists, and also estimate the

degree of convergence of the sequence of solutions of the difference equation. It is not necessary to compute a itself since 2^a appears in (2.5.1). We wish to emphasize once more, that the considerations of this section are not rigorous.

3. Specific Problems Considered

In order to obtain some indication as to the validity of the non-rigorous mathematical considerations of the previous section, we have solved some sample problems on the Ordvac computer at Aberdeen. We chose problems involving either boundary conditions (2.1.1) or (2.1.2) and either linear and non-linear differential equations. Actually, as will be seen in the next section, the program which was prepared for Ordvac is capable of handling entire classes of problems rather than merely the specific problems described below.

3.1. Boundary value problem - linear differential equation (BVL). Here we selected a problem for which an analytic solution is readily available. The equations are

$$(3.1.1) \quad \begin{cases} u_t = u_{xx} & , \quad 0 < x < 1, \quad t > 0, \\ u(x,0) = g(x) & , \quad 0 < x < 1 \\ u(0,t) = u(1,t) = 0 & , \quad t \geq 0. \end{cases}$$

The analytic solution for the case $g(x) = 1$ is given by

$$(3.1.2) \quad u(x,t) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin nx e^{-n^2 \pi^2 t}$$

We shall, by solving the difference equations with various mesh sizes, attempt to determine the rate of convergence for both methods. For the Crank-Nicolson method we shall let $k = O(h)$ as $h \rightarrow 0$, even though the theoretical results have been proved only under stronger restrictions on k , [13], in an attempt to determine whether a generalization is to be expected.

3.2. Boundary value problem - non-linear differential equation (BVP).

The following problem described by Hartree [7] appears to be typical of this class of problems.

$$(3.2.1) \quad \begin{cases} u_t = u_{xx} + \gamma e^u & 0 < x < 1, \quad t > 0 \\ u(x,0) = 0 & 0 < x < 1 \\ u(0,t) = u(1,t) = 0 & t \geq 0 \end{cases}$$

Here $u(x,t)$ represents the temperature in a substance where there is generation of heat increasing exponentially with the temperature. When γ exceeds a certain critical value there is no steady state solution and the solution increases beyond all bounds. We shall not study this aspect of the problem but, rather, will use a fixed value of 0.8 for γ , which is below the critical value. We shall solve the problem by the forward Difference and Crank-Nicolson method for several values of h . Solutions for various values of γ have been obtained by Hartree using a differential analyzer and the results agreed quite well with experiments.

3.3. Normal derivative problems (NDL and NDN). Here we consider boundary conditions (2.1.2) with both the linear equation

$$(3.3.1) \quad u_t = u_{xx} \quad 0 < x < 1, \quad t > 0$$

and the non-linear equation

$$(3.3.2) \quad u_t = u_{xx} + e^{-1/u}, \quad 0 < x < 1, \quad t > 0.$$

The initial conditions are

$$(3.3.3) \quad f(x) = c \quad 0 \leq x \leq 1$$

where in the cases which we shall consider $c = .031$. Actually, in our computations, we shall take for our initial function not $f(x) = .031$ but a set of

values obtained for a later value of t using the analytic solution of the linear problem (see for instance [8], page 22). The values are given in Table I. Even in the non-linear case, these values are sufficiently accurate since the non linear term is negligible for small values of t . This adjustment in the initial conditions was made to eliminate any possible effect of the singularity caused by the discontinuity of u_x when $t = 0$. It is by no means certain that such a precaution would be necessary, and for the linear case at least, it should be possible to determine analytically the effect of the singularity.

Problems of this type involving (3.3.1) are designated NDN and those involving (3.3.2) are designated NDN. For NDN problems the solution $u(x,t)$ represents the temperature in a propellant where the reaction rate is determined by the Arrhenius term $e^{-1/u}$. The propellant is assumed to be a semi-infinite slab, $0 \leq x < \infty$. The propellant is heated by a gas at temperature u_g which occupies the region $x < 0$ and whose influence on the propellant depends on the heat transfer coefficient h . In order to be able to use finite difference methods we consider a slab of finite thickness A and replace the condition $\lim_{x \rightarrow \infty} u_x = 0$ by the condition (2.1.2b). Further details on the physical motivation for these problems may be found in [8].

In order to represent more accurately the physical situation, it was sometimes necessary to introduce "shutoff"; that is after a certain value of t , u_g is greatly reduced. However, we shall not do this in our study.

We shall also not consider the determination of the "ignition time" which is the time required for the value of $u(x,t)$ to increase above a preassigned value.

We shall assume the following values for the parameters

$$A = 73,600$$

$$c = .031$$

$$\frac{u}{g} = .18$$

$$H = 2 \times 10^{-6}$$

Prior to 1952 a number of calculations were done on this problem at the Aberdeen Proving Ground using the Bell Relay Computer and the Eniac. The Forward Difference method was used with $r = \frac{1}{2}$ and several values of h . We shall make use of some of these results in Section 5.

4. Description of the Program for Drives

To run a particular problem with the program as presently coded, it is necessary to specify three major conditions; i.e. (1) the difference equation to be used, (2) the boundary conditions, and (3) the necessary parameters such as h , r , etc.

All of the difference equations and boundary conditions described in Section 2 have been coded and any problem involving these can be computed using the program. Except for the CNF method, the interior points of the $(j+1)$ st row are computed followed by the computation or insertion of the boundary values of that row. This permits the boundary conditions to be easily modified. The appendix contains the detailed equations used in the present coding.

Unless otherwise instructed, the machine will assume that the differential equation is linear. In the non-linear case it is necessary to instruct the machine to compute the non-linear term.

For the DS method, since the j -th and $(j-1)$ st rows are necessary to compute the $(j+1)$ st row (see appendix), it was necessary to compute the first row by a different method. We used the sD method. The number of rows necessary to be computed by the sD method depends upon r , which involves k , the increment in time. This is noted in the Appendix.

For the CN method, NDW case, when the values of the function became large, the iterative scheme would not converge. A feature was added in the program whereby if the number of iterations exceeded a given K_0 for the $(j+1)$ st row, the coding would revert back to the sD method and continue computation from the j -th row using r' , where $r = r' \cdot 2^k$ and $0 < r' \leq \frac{1}{2}$.

Shutoff, another feature, can be described as reducing the gas temperature

(u_g) or shutting off the gas flow after time t_g (see Section 3). After computing j_g rows (ND only), the value of u_g can be changed for the (j_g+1) st row and the remaining rows.

The parameters that must be chosen are:

$$b = \Delta x / \Delta$$

$$r = k/h^2$$

S switch - which is the stopping procedure where $S = S_1$ stops the machine after m rows and $S = S_2$ stops machine when $\max |u_{i,j}|$ exceeds or falls below a given tolerance.

Besides these parameters, certain specific cases will require a specification of other information, such as:

$x_0(\text{CN})$ - as explained above

$\omega(\text{CN})$ - the relaxation factor. If ω is not specified, $\omega = 1$ is assumed

$\gamma(\text{EVN})$: (.8 was used)

$H(\text{ND})$: $(2 \cdot 10^{-6}$ was used)

$u_g(\text{ND})$: (.18 was used)

$\Delta(\text{ND})$: (73,600 was used)

$j_g, u_g^{(1)}$ (ND) - (shutoff); replaces u_g by $u_g^{(1)}$ after computing j_g rows.

The non-linear term was computed by a floating point subroutine with the exponential factor being computed by taking the first 15 terms of the series expansion of e^x . Initially, the exponent was normalized; i.e. placed in the form $a \cdot 2^k$ where $\frac{1}{2} \leq |a| < 1$, or $a = 0$ where appropriate. (For the RV cases, $a = 4$ since all values were scaled by 2^{-4} . For ND cases, the presence of the exponent $(-\frac{1}{m})$ necessitated

the normalizing procedure.) Then, $2^{-2}e^{\alpha}$ was computed followed by a normalization of e^{α} . Since $e^{f(u)}$ was desired, the scaling problem was solved by the following:

$$e^{f(u)} = e^{\alpha \cdot 2^{\alpha}} = (e^{\alpha})^{2^{\alpha}}$$

Therefore, it was necessary to square e^{α} a times in computing the non-linear term.

5. Analysis of Results

In Tables II - IX we give the values of $u(x,t)$ for the respective problems as obtained by the various finite difference methods. Scaling factors are indicated on the tables. In each case the columns headed FD($\frac{1}{2}$) and FD($\frac{1}{4}$) contain results obtained using the Forward Difference method with $r = \frac{1}{2}$ and $r = 1/4$, respectively. Columns headed CN(I) and CNN(I) contain the results obtained by using the Crank-Nicolson method using the iterative and non-iterative numerical procedures, respectively. For different values of $M = A/h$, the following values of r are used

<u>M</u>	<u>r</u>
8	1/2
16	1
32	2
64	4

The column headed CNN(II) contains results obtained using the Crank-Nicolson method, non-iterative and with the following values of r

<u>A/h</u>	<u>r</u>
8	1
16	2
32	4
64	8

The value of t can be obtained from the row number by multiplying the row number by $\frac{1}{128} A^2$. Thus the row number equals t/k_8 where k_8 is the value of k corresponding to $M = 8$ and $r = 1/2$. The column headed "Eniac" gives results obtained on the Eniac using the Forward Difference method and $r = 1/2$.

Corresponding to each of the row numbers 4, 8, 12, 16, and 20 and to the indicated values of x/A we give the following results, when available,

M	u_M
8	u_8
	*
16	u_{16}
	*
32	u_{32}
	*
64	u_{64}
	*
	[x]

Here u_M represents the solution of the difference equation being considered with $h = 1/M$. Also, $e_{16} = u_{16} - u_8$, $A = e_{16}/e_{32}$, $B = e_{32} = u_{32} - u_{16}$, $C = e_{32}/e_{64}$, and $D = e_{64} = u_{64} - u_{32}$. In the brackets we give the extrapolated value. The estimated value of ρ used in the extrapolation is given at the bottom of the column, (see section 2.5). For the extrapolation e_{64} is used when available, otherwise e_{32} is used. An asterisk in place of $e_{M/2}/e_M$ indicates that the computed value is not regarded as significant, usually because e_M is too small. An asterisk near an extrapolated value means that the value obtained from the use of the smallest mesh size is given in place of the extrapolated value.

5.1. Boundary value linear (BVL). In this case the results obtained from the Crank-Nicolson method with the iterative and the non-iterative numerical procedures were identical. Since the ratios e_M/e_{2M} are close to 4 it would appear that $e_M = O(M^{-2})$ and that extrapolation to zero grid size based on $\alpha = 2$ might give good results. Indeed, if one uses this procedure one obtains almost identical results for all methods and very close agreement with the exact value as calculated from (3.3.2). We note that the values obtained from the Forward Difference method with $r = \frac{1}{2}$ and $\lambda = 32$ are considerably different

from the exact values and that the extrapolation process has greatly improved the accuracy. We also remark that for this particular problem the Crank-Nicolson method is much more accurate than the Forward Difference method although the extrapolated values are practically the same.

5.2. Boundary value non-linear (BVM). As in the linear case the values of e_M/e_{2M} are, with the FD and CN methods, close to 4. Extrapolation to zero grid size using $\rho = 4$ and $\alpha = 2$ yields results which are nearly the same for both the FD method (with $r = \frac{1}{2}$ as well as with $r = 1/4$) and for CN(I). On the other hand with the non-iterative procedures CNN(I) and CNN(II), (where the less accurate difference equation obtained by replacing f_2 by f_0 in (2.3.2) was used), the values of e_M/e_{2M} were usually between 3 and 3.5. Thus as expected, the order of convergence was less than for the other methods. Nevertheless with an extrapolation using $\rho = 3$ we obtained fairly accurate results, especially for CNN(I).

We believe that combining CNN with a few iterations, not more than five, would increase the order of convergence.

The error due to using f_0 instead of f_2 in (2.3.2) varies approximately as K^{-1} as can be seen from comparing results of CN(I) and CNN(I). Thus for the 10th row and for $x = \frac{1}{2}$ we have

M	CN(I)	CNN(I)	CN(I)-CNN(I)
8	72534	72400	134
16	72888	72821	67
32	72977	72943	34

(All values have been multiplied by 10^5 .)

Examining the differences 134, 67, 34 we observe that they are approximately in the ratios 4:2:1. Hence the differences appear to tend to zero like M^{-1} . This tends to confirm our prediction that the error introduced by using the less accurate difference equation is of order M^{-1} .

5.3. Normal derivative linear (NNL). In both the linear and the non-linear cases we are concerned with three options for representing the condition (2.1.2a). We first consider the results obtained for the linear case for Options I, II, III as given in Tables IV, V, VI respectively. As in the boundary value linear case it did not matter whether one used the iterative or the non-iterative procedure for the Crank-Nicolson method.

For Option I the values obtained by the Forward Difference method for $r = 1/4$ and $r = 1/2$ agree closely with each other and with those obtained with CNN(I) and CNM(II). Based on the observed value of ρ , extrapolated values were obtained as indicated. Of course, in this case we can conclude little from the fact that the extrapolated values obtained from the different methods agree with each other. However, the extrapolated values do agree rather closely with those obtained from results using Option II and III, and the latter two agree with each other. Moreover, the difference $u_{64} - u_{32}$ obtained for CNM(I) with Option III was very small, and this indicates that u_{64} is probably very close to the true value of u . Thus it would appear that in this case (2.1.5) (Option I) is a reasonably satisfactory representation of (2.1.2a) provided one uses the proper extrapolation procedure.

Finally we compare our results with the "exact" values obtained under the assumption that A is infinite, using the procedure given in [8]. These values are given on Table IV in braces. Near the line $x = A$ our values will not agree

with these "exact" values, because in our case A is finite. Nevertheless the agreement is generally rather close.

We give in Table V the values obtained on the Eniac using Option II and the FD method with $r = \frac{1}{2}$. Although the Eniac values and the Ordvac values listed under FD, again with $r = \frac{1}{2}$, agree exactly for $M = 8$, exact agreement cannot be expected for other values of M . The reason for this is that $A=64,400$ was used for the Eniac results instead of $A=73,800$ as used on the Ordvac. On the Eniac, instead of (2.1.14), the condition

$$u_2 = u_{M+1}$$

was used to represent (2.1.2b). Thus, since $64,400/73,800 = 7/8$ we have exact agreement in the case $M = 8$.

Near the left hand boundary, ρ appears to be rather close to 4.0 so that we use extrapolation based on $a = 2$. We note that $u_{32} - u_{16}$ is small, and this indicates that u_{32} is already quite accurate. For $x/A = \frac{1}{2}$ the use of $\rho = 3$ seems indicated, and for $x/A = 1$ we used $\rho = 2$. It appears that the largest errors occurred at the right hand boundary.

Similar results were obtained for Option III as indicated in Table V. Of course for Option III it was possible to use CWN(I) and thus use many fewer time steps than were necessary for the Forward Difference method.

It seems reasonable to suppose that, by using either (2.1.15) or (2.1.17) to represent more accurately the right hand boundary condition, and by using Option III or III', the ratio ρ would be nearly 4 everywhere and that extrapolation based on $a = 2$ could have been used for all points.

5.4. Small derivative non-linear (MDN). The Eniac results obtained

using the FD method for Option II indicate that extrapolation to zero grid size using $\alpha = 2$ for $x/A = 0, 1/4$ and $\alpha = 1$ for $x/A = 1/2, 1$ should be quite accurate. The same also appears to be true for our Ordvac results. Of course the extrapolated values obtained in the respective cases do not agree because of the difference in the boundary conditions at $x/A = 1$, as mentioned above. The extrapolated values obtained on the Ordvac using Option II and the FD method also agree very closely with those extrapolated values obtained using CN(1) with Option III. It is difficult to make definite statements as to the behavior of the CNN method except that the errors are small and irregular. Here, of course, Option III' was used.

For Option I the ratios ρ are all approximately 2 with all difference equations as in the linear case. The errors are somewhat larger and the extrapolated values somewhat less accurate than with Option III.

5.5. Machine times. Figures 5 and 6 show the approximate times required to compute $t = 10k_3$ rows by the various methods in both the linear and in the non-linear cases respectively. The times for BV problems and for ND problems were nearly the same. The slopes for the curves corresponding to the FD, CN and CNN methods, after proper corrections have been made to account for the use of different logarithmic bases, are approximately 3, 5/2, and 2 respectively. Hence as expected, the times increase as k^3 , $k^{5/2}$ and k^2 respectively. For the non-linear cases about 10 times as much machine time was required as for the linear cases.

The number of iterations required using the Crank-Nicolson method seemed to be nearly independent of whether the differential equation was linear or non-linear or whether BV or ND boundary conditions were used. The following

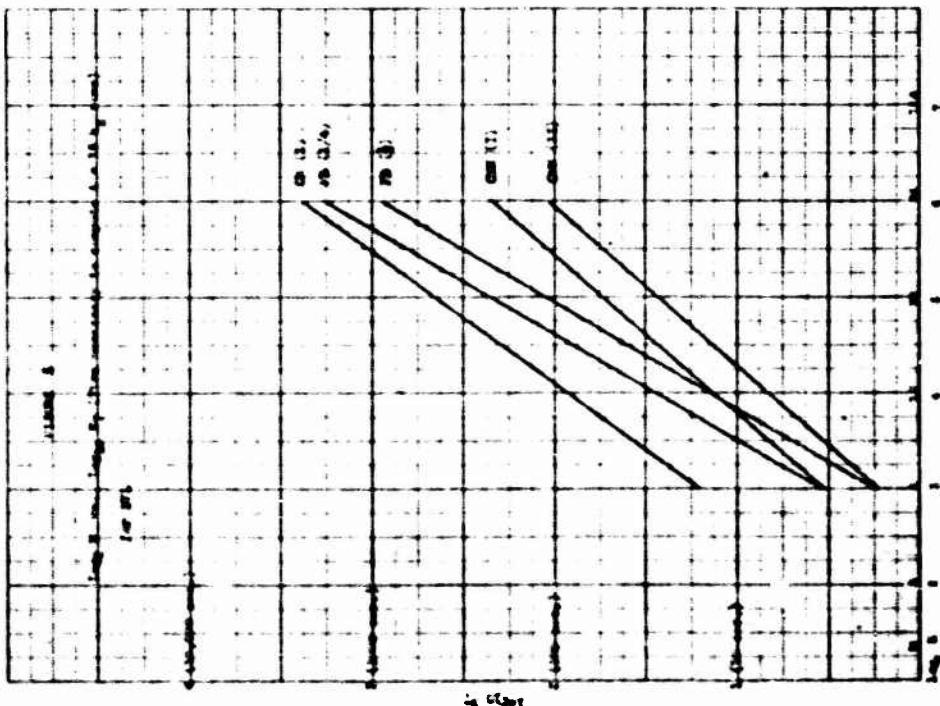
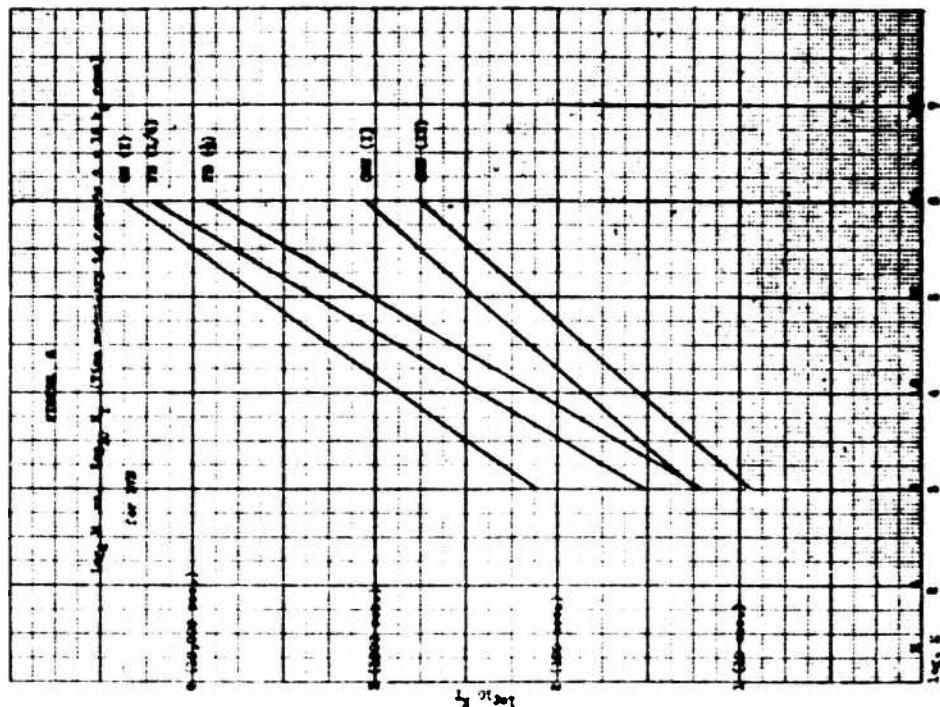


Table gives the value of ω used for each M and the approximate number of iterations required per row.

<u>M</u>	<u>ω</u>	<u>No. of Iterations</u>	
		<u>Per Row</u>	
8	1.025	8	
16	1.069	11	
32	1.144	15	
64	1.375	20	

5.6. Tentative conclusions. Considering the analysis of the results as a whole we are led to the following tentative conclusions:

1. In the linear case, the error caused by the use of any of the difference equations rather than the differential equations varies as h^2 . In the non-linear case this is true for the FD and CN methods but for the CNN(I) and CNN(II), the error varies as h .
2. The use of Option I and the condition (2.1.14) used at $x/A = 1$ introduce errors of order h . On the other hand, the use of Option II, when it can be used, and Options III and III' introduces errors of order h^2 .

Further work should include the following:

1. In the non-linear cases, BVM and KMM, try CNN with a fixed number of iterations independent of h .
2. For KMM use CNN with Option III' for the left hand boundary condition and (2.1.15) or (2.1.17) to represent the right hand boundary conditions.

5.7. Differential method. We have not given the results which were obtained using the DIF method. The results which were obtained indicated that the method could not be as effective as the CN or CNN method. However, this should be studied further both analytically and by running some cases on the

machine. Results obtained in [5] indicate that one must require that $k = o(h)$ in order to obtain convergence, and that, moreover, the order of convergence is dependent on the order of h/k as $h \rightarrow 0$. Also, the fact that a special procedure appears to be needed to start the process is a disadvantage of the method.

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List of Abbreviations

1. Differential Equations and Boundary Conditions

Symbol	The function $f(x,t,u)$ in (1.1)	Boundary conditions
HVL	0	See (3.1.1) with $g(x)=1$.
FVM	u^{α}	See (3.2.1).
NDL	0	See (2.1.2).
NDN	$e^{-t/u}$	See (2.1.2).

For both NDL and NDN the initial values used are given in Table I.

2. Difference Equations

FD Forward Difference

$$\begin{aligned} FD\left(\frac{1}{2}\right) &\text{ uses } r = \frac{1}{2} \\ FD\left(\frac{1}{4}\right) &\text{ uses } r = \frac{1}{4} \end{aligned}$$

CN Crank-Nicolson (iterative)

CN(I) uses $r = \frac{1}{2}, 1, 2, 4$ with $N = 8, 16, 32, 64$, respectively.

CNN Crank-Nicolson (non-iterative)

CNN(I) uses $r = \frac{1}{2}, 1, 2, 4$ with $N = 8, 16, 32, 64$ respectively.

CNN(II) uses $r = 1, 2, 4, 8$ with $N = 8, 16, 32, 64$ respectively.

DFD Dubort-Frankel

3. Representations of (2.1.2a) - (for ND problems only)

Option	Equation
I	(2.1.5)
II	(2.1.7)
III	(2.1.11)
III'	(2.1.13)

TABLE I

Initial values for MD cases
(M = 64)

x/A	$u_{1,0} \cdot 10^7$	x/A	$u_{1,0} \cdot 10^7$	x/A	$u_{1,0} \cdot 10^7$
0	*** 34304	3/8	• 31123	3/4	** 31000
	33980		31100		31000
	* 33677		*** 31081		* 31000
	33395		31065		31000
	** 33134		* 31052		*** 31000
	32894		31041		31000
	* 32674		** 31033		* 31000
	32473		31026		31000
	1/8 *** 32290		* 31020		** 31000
	32125		31016		31000
1/8	* 31977	1/2	*** 31012	7/8	* 31000
	31844		31009		31000
	** 31726		* 31007		*** 31000
	31621		31005		31000
	* 31529		** 31004		* 31000
	31449		31003		31000
	1/4 *** 31378		* 31002		** 31000
	31318		31002		31000
	* 31265		*** 31001		* 31000
	31220		31001		31000
1/4	** 31182	1	* 31001	1	*** 31000
	31150		31001		

• - M = 32

** - M = 32, 16

*** - M = 32, 16, 8

TABLE II
SOLUTIONS OF DIFFERENCE EQUATION FOR BVL
(All values multiplied by 10^5 .)

$x = 1/4, 3/4$									
Row	n	$FD(3)$	$FD(4)$	$CW(I)^\circ$	$CW(II)^\circ$	$FD(3)$	$FD(4)$	$CW(I)$	$CW(II)$
	8	17520	18023	19376	19333	24777	26619	27302	27341
	16	1303	328	-54	-54	1842	464	-71	-71
20	16	16823	19151	19279	26619	27003			
	32	$3.97/328$	$4.0/82$	$3.86/-14$	$3.97/464$	$4.0/116$			
	EXACT	[19260]	[19260]	[19260]	[19260]	[27238]	[27238]	[27238]	[27238]
	8	24048	25674	26278	26230	34009	36081	37158	37091
	16	1626	409	-44	-8	2299	801	-80	-71
12	16	25674	26083	26234	26222	36308	36885	37099	37082
	32	$3.98/409$	$4.0/102$	$4.0/-11$	$4.0/-2$	$3.98/577$	$5.5/145$	$3.8/-16$	$2.75/-4$
	EXACT	[26219]	[26219]	[26219]	[26219]	[37071]	[37070]	[37070]	[37070]
	8	33008	35023	35647	35588	46680	49520	50377	50336
	16	2015	506	81	81	2840	708	113	113
12	16	35023	35529	35669	35669	49520	50228	50329	50329
	32	$3.98/506$	$3.93/127$	$3.68/22$	$4.01/708$	$4.0/177$			
	EXACT	[35698]	[35698]	[35698]	[35698]	[50404]	[50405]	[50459]	[50459]
	8	45312	47839	48485	48322	61063	67451	68314	68125
	16	2527	646	278	278	3388	822	321	321
8	16	47839	48485	48600	48600	67451	68273	68352	68352
	32	$4.0/630$	$3.99/162$	$3.48/80$	$4.12/822$	$4.0/248$			
	EXACT	[48678]	[48691]	[48688]	[48688]	[68273]	[68477]	[68529]	[68522]
	4	62500	66534	67501	66330	87500	90192	92783	93477
	16	40346	1095	1517	1517	2692	537	370	370
4	16	66534	67629	67847	67847	90192	90729	90857	90857
	32	$3.68/1095$	$3.95/277$	$31.87/102$	$5.01/537$	$4.28/123$			
	EXACT	[67629]	[67994]	[67982]	[67943]	[90908]	[90909]	[90920]	[90920]
	8	b	b	b	b	b	b	b	b
	4	b	b	b	b	b	b	b	b
	16	b	b	b	b	b	b	b	b
	32	b	b	b	b	b	b	b	b
	EXACT	[67994]	[67994]	[67977]	[67977]	[90908]	[90909]	[90920]	[90920]

* - see Section 5

TABLE III
SOLUTIONS OF DILUTE SULFURIC ACID
(ALL VOLUMES REFERRED TO 20° C.)

TABLE IV

SOLUTIONS OF DIFFERENCE EQUATIONS FOR POL. OPTICS Z.
(All values multiplied by 10^{-6} .)

		$x/\lambda = 0$				$x/\lambda = \frac{1}{2}$				$x/\lambda = \frac{3}{2}$			
Row	N	PD(r=0)	PD(r=1)	CWN(I)	CWN(II)	PD(r=0)	PD(r=1)	CWN(I)	CWN(II)	PD(r=0)	PD(r=1)	CWN(I)	CWN(II)
23	8	41833	41837	41835	41839	37176	37204	37256	37240	36183	36205	36203	36201
	16	-524	-531	-518	-499	-336	-315	-335	-316	-136	-223	-214	-197
	32	41309	41306	41292	41290	36810	36838	36811	36826	33989	33922	33929	33926
	64	-1057-255	-2.1/-247	2.06/-246	2.05/-164	2.12/-158	2.08/-153	2.06/-95	2.13/-96	2.11/-92	2.12/-75	2.13/-71	2.13/-68
	128	41054	41050	41048	41046	36676	36673	36672	36674	33836	33833	33832	33830
	Exact	[40799] [40803]	[40804] [40806]	[40805] [40807]	[40806] [40808]	[36513] [36515]	[36522] [36524]	[36521] [36523]	[36520] [36522]	[33797] [33799]	[33798] [33799]	[33803] [33805]	[33804] [33806]
24	8	40941	40943	40942	40943	36296	36308	36252	36250	31448	31571	31570	31568
	16	-519	-526	-509	-488	-307	-317	-304	-283	-146	-166	-168	-151
	32	40422	40417	40408	40402	35907	35905	35976	35969	33302	33375	33378	33377
	64	-106-252	2.1/-250	2.1/-262	2.06/-237	0.05/-150	2.14/-146	2.14/-134	2.14/-131	.97/-76	2.16/-77	2.16/-75	2.13/-71
	128	40170	40169	40166	40168	35837	35832	35834	35832	33279	33278	33277	33276
	Exact	[39918] [39920]	[39919] [39921]	[39920] [39922]	[39921] [39923]	[35687] [35691]	[35689] [35693]	[35685] [35687]	[35686] [35688]	[33157] [33160]	[33151] [33153]	[33152] [33154]	[33153] [33155]
25	8	39937	39939	39908	39875	35319	35329	35304	35272	32709	32735	32736	32733
	16	-514	-520	-501	-476	-270	-263	-266	-262	-76	-123	-121	-108
	32	39443	39419	39407	39399	35049	35047	35038	35030	32614	32617	32615	32609
	64	-0.07/-248	2.11/-216	2.1/-237	2.1/-231	0.06/-131	2.16/-130	2.12/-128	2.1/-114	1.81/-52	2.19/-51	2.18/-53	2.17/-48
	128	39175	39173	39170	39168	34918	34917	34914	34912	32562	32563	32564	32562
	Exact	[38927] [38929]	[38927] [38929]	[38929] [38931]	[38931] [38933]	[34787] [34791]	[34787] [34791]	[34784] [34786]	[34785] [34787]	[32510] [32509]	[32502] [32504]	[32512] [32514]	[32511] [32513]
26	8	38735	38759	38776	38683	34200	34216	34190	34151	31973	32006	32012	32009
	16	-503	-510	-490	-459	-211	-226	-217	-192	-36	-51	-76	-53
	32	38242	38249	38236	38223	33299	33298	33278	33269	31937	31932	31931	31936
	64	2.01/-260	2.13/-239	2.7/-226	2.06/-220	0.03/-156	2.2/-103	2.7/-75	2.05/-39	1.49/-76	2.13/-59	2.44/-29	2.04/-26
	128	38012	38010	38006	38004	33085	33085	33082	33080	31911	31912	31912	31910
	Exact	[37772] [37780]	[37772] [37780]	[37784] [37786]	[37784] [37786]	[33781] [33782]	[33782] [33783]	[33781] [33782]	[33780] [33781]	[31805] [31807]	[31807] [31808]	[31806] [31807]	[31805] [31806]
27	8	37267	37262	37220	37168	32844	32883	32862	32806	31306	31363	31363	31359
	16	-467	-484	-460	-416	-99	-129	-117	-73	26	-3	-23	-13
	32	36780	36778	36760	36766	32751	32758	32745	32731	31330	31332	31330	31337
	64	0.12/-220	2.2/-219	2.2/-206	2.1/-196	1.69/-55	2.77/-50	2.79/-51	1.78/-42	0/-1	1.13/-5	2.08/-8	2.6/-5
	128	36560	36559	36558	36550	32696	32694	32491	32491	31338	31332	31330	31338
	Exact	[36347] [36361]	[36347] [36360]	[36356] [36357]	[36357] [36358]	[32741] [32742]	[32741] [32742]	[32740] [32741]	[32740] [32741]	[31330] [31331]	[31329] [31330]	[31329] [31330]	[31329] [31330]
28	2	2	2	2	2	2	2	2	2	2	2	2	2

TABLE IV

SOLUTIONS OF DIFFERENCE EQUATIONS FOR μ_{ex} , OPTION L
(All values multiplied by 10^{-3} .)

	$x/b = \frac{1}{2}$				$x/b = 1$			
	$P_0(r-\frac{1}{2})$	$C_{\text{HW}}(\text{I})$	$C_{\text{HW}}(\text{II})$		$P_0(r-\frac{1}{2})$	$P_0(r+\frac{1}{2})$	$C_{\text{HW}}(\text{I})$	$C_{\text{HW}}(\text{II})$
76	37184	37156	37140		36183	36205	36203	36201
76	-345	-335	-316		-194	-213	-214	-197
76	36838	36831	36824		33969	33932	33969	33956
-168	2.12/-158	2.08/-152	2.04/-152		2.04/-95	2.04/-95	2.04/-96	2.04/-92
76	36673	36672	36672		33973	33952	33952	33952
	2.00/-76				2.04/-45			2.04/-49
	36597				33948			33941
	[36521]	[36520]			[33929]	[33900]		[33924]
74	36308	36280	36252		33448	33473	33468	33467
77	-317	-306	-283		-116	-166	-158	-151
71	35945	35976	35949		33302	33325	33302	33312
50	2.11/-114	2.11/-114	2.11/-113		2.11/-76	2.11/-77	2.11/-75	2.11/-71
	X331	35831	35832		33229	33229	33227	33226
	2.06/-59				2.11/-35			2.11/-33
71	[35639]	[35639]	[35639]		[33151]	[33151]	[33151]	[33150]
51								
9	35378	35354	35372		32798	32735	32736	32733
9	-262	-262	-262		-76	-123	-123	-118
9	35047	35038	35030		32614	32617	32615	32609
11	2.16/-136	2.16/-136	2.16/-136		2.16/-59	2.16/-59	2.16/-59	2.16/-59
	34921	34914	34912		32562	32563	32562	32561
	2.07/-40				2.12/-25			2.12/-25
	34852				32532			32531
71	[34767]	[34767]	[34767]		[32510]	[32502]	[32512]	[32511]
34216	34190	34151			31971	32036	32032	32039
-228	-212	-182			-76	-54	-78	-53
33968	33978	33959			31931	31952	31931	31930
2.27/-103	2.27/-76	2.07/-29			2.12/-36	2.12/-36	2.12/-36	2.12/-36
33805	33802	33800			31911	31912	31912	31910
2.09/-16					2.07/-11			2.07/-11
	33936				31890			31879
63762	[33730]	[33731]			[31885]	[31887]	[31889]	[31887]
32883	32862	32856			31106	31124	31123	31120
-129	-117	-73			-76	-9	-23	-13
32754	32725	32733			31132	31132	31132	31130
7.71/-58	7.29/-51	1.71/-42			1.11/-5	2.04/-8	2.4/-5	1.11/-3
32636	32636	32631			31132	31132	31132	31130
2.11/-28					2.67/-3			2.67/-3
	32670				31132			31130
7.34/-36	[32646]	[32646]			[31130]	[31129]	[31129]	[31129]
2	2	2			2	2	2	2

TABLE V

 SOLUTIONS OF DIFFERENCE EQUATIONS FOR NDL, OPTION II ($\lambda = \frac{1}{2}$)
 (All values multiplied by 10^6 .)

Row	N	$x/4 = 0$			$x/4 = \frac{1}{2}$			$x/4 = 1$		
		ENIAC	FD(3)	CM(3)	ENIAC	FD(3)	CM(3)	ENIAC	FD(3)	CM(3)
20	8	40052	40052			36560	36567		33815	
	16		-30			-27			-24	
	32		40022		36533			33821		
	8		3.3/-9		3.85/-7			2.66/-9		
	16		40013		36526			33812		
	32		[40010]		[36524]			[33808]		
16	8	39973	39973	39948		35730	35730	35714	33177	33177
	16	-29	-29	-32		-17	-17	-24	16	-11
	32	39944	39941	4.0/-8		35713	35708	35703	33193	33166
12	8	38987	38987	38959		34826	34826	34808	32516	32516
	16	-34	-34	-35		-21	-22	-22	32525	-1
	32	38952	38953	4.4/-8		34805	34804	34798	32515	1.0/-1
	8						3.67/-6		32514	
	16						34798		[2516]	
	32						[34796]			
8	8	37838	37838	37809		33817	33817	33801	31876	31876
	16	-37	-37	-37		-19	-19	-19	31885	31883
	32	37801	37801	4.1/-9		33798	33798	33791	31885	3.5/2
4	8						3.8/-5		31895	
	16						33791		[31886]	
	32						[33793]			
1	8	36414	36414	36387		32662	32662	32654	31306	31306
	16	-60	-60	-60		-12	-12	-12	31322	16
	32	36378	36378	4.0/-10		32650	32650	32648	31322	5.0/3
	8						6.0/-2		31325	
	16						32648		[31328]	
	32						[32647]			
• - see Section 5										

TABLE V

S OF DIFFERENCE EQUATIONS FOR KDL, OPTION II ($\alpha = \frac{1}{2}$)(All values multiplied by 10^6 .)

		$x/A = \frac{1}{2}$				$x/A = \frac{1}{2}$	
ENIAC	FD(?)	CM(?)		ENIAC	FD(?)	CM(?)	
	35560	35571			33845		
	-27				-26		
	36533				33821		
	3.85/-7				2.66/-9		
	36526				33812		
	(36524)				[33808]		
	35730	35714			33177	33192	
	-17				16	-11	
	35723				33193	33166	
						2.8/-4	
						33162	
						[33160]	
	34826	34808			32516	32533	
	-21				9	-1	
	34805				32525	32515	
						1.0/-1	
						32514	
						[32517]	
	33817	33801			31876	31876	
	-19				9	7	
	33798				31885	31883	
						3.5/2	
						31895	
						[31888]	
	32662	32654			31306	31306	
	-12				6	16	
	32650				31322	31322	
						5.0/3	
						31325	
						[31328]	

TABLE VI

SOLUTIONS OF DIFFERENCE EQUATIONS FOR KEL. OPTION III
(all values multiplied by 10^6 .)

		x = 0		x = 1		x = 2		x = 3	
Row	N	FD(3)	CWN(1)	FD(4)	CWN(1)	FD(3)	CWN(1)	FD(4)	CWN(1)
20	8	40832	40781	36521	36508	33820	33816	32198	32246
	16	40835	40808	36529	36521	33818	33818	32175	32170
	32	40835	40813	36529	36523	33818	33811	32063	32076
	64	40813	40810	36529	36523	33811	33807	32063	32076
			[40810]		[36523]		[33807]		[32076]
16	8	39917	39893	35690	35676	33152	33170	31726	31776
	16	39917	39917	35701	35697	33161	33161	31636	31647
	32	39916	39921	35697	35697	33161	33161	31535	31535
	64	39932	39928	35699	35696	33161	33150	31572	31572
			[39931]		[35697]		[33150]		[31549]
12	8	38924	38836	31766	31768	32198	32515	31318	31397
	16	38914	38931	31779	31789	32523	32521	31302	31313
	32	38914	38930	31779	31789	32523	32521	31278	31281
	64	38914	38930	31779	31775	32523	32511		31281
			[38914]		[31779]		[32511]		[31253]
8	8	37766	37737	32732	33765	31164	31895	31101	31139
	16	37792	37775	33773	33784	31162	31895	31089	-12
	32	37792	37775	33773	33784	31162	31895	31089	31077
	64	37790	37785	33792	33789	31165	31895	31081	1.5/-8
			[37789]		[33792]		[31895]		3.0/-15
4	8	36337	36305	32642	32631	31106	31134	31006	31019
	16	36363	36312	32647	32642	31132	31136	31007	-9
	32	36363	36367	32647	32642	31132	31136	31007	31010
	64	36363	36367	32647	32646	31132	31137	31006	3.0/-3
			[36364]		[32646]		[31137]		[31006]
P		A		B		C		D	

TABLE VII

SOLUTIONS OF DIFFERENCE EQUATIONS FOR \sin , SECTION 1.
(All values multiplied by 10^6 .)

		$n/4 = 0$				$n/4 = \frac{1}{2}$				$n/4 = 1$				
Row	N	PD($r_{n/4}$)	PD($s_{n/4}$)	CHE(I)	CHE(II)	CHE(I)*	CHE(II)*	PD($r_{n/4}$)	PD($s_{n/4}$)	CHE(I)	CHE(II)	CHE(I)	CHE(II)	PD($r_{n/4}$)
20	8	13615	13853	13821	13805	13805	13805	13816	13816	13816	13816	13816	13816	13816
	16		2970	1211	1211	1211	1211	13842	13842	13842	13842	13842	13842	13842
	32		58821	13638	13807	13807	13807	13842	13842	13842	13842	13842	13842	13842
	64			0.37/3803	0.38/1730	0.37/3803	0.38/1730	0.37/3803	0.38/1730	0.37/3803	0.38/1730	0.37/3803	0.38/1730	0.37/3803
16	8	41253	41595	41595	41595	41595	41595	41595	41595	41595	41595	41595	41595	41595
	16	-168	-196	-193	-70	-191	-218	-748	-773	-180	-742	-180	-150	-158
	32	41391	41601	41601	41601	41601	41601	41601	41601	41601	41601	41601	41601	41601
	64	2.3/-71	4.2/-44	2.7/-71	1.8/-119	2.7/-71	1.8/-119	2.19/-105	2.18/-84	1.76/-48	1.38/-58	1.17/-59	2.0/-66	31631
12	8	40160	40176	40117	40048	40149	40149	40149	40149	40149	40149	40149	40149	40149
	16	-396	-110	-388	-354	-375	-239	-257	-239	-205	-246	-211	-36	-118
	32	39766	39756	39729	39696	39756	39756	39756	39756	39756	39756	39756	39756	39756
	64	0.6/-193	2.22/-175	2.75/-157	1.96/-172	2.75/-157	1.96/-172	2.15/-111	2.05/-108	1.75/-49	1.30/-50	2.18/-44	2.06/-31	31296
8	8	39573	39730	39730	39554	39532	39532	39532	39532	39532	39532	39532	39532	39532
	16			2.36/-76	39730	39730	39730	39532	39532	39532	39532	39532	39532	39532
	32			[39360]	[39360]	[39360]	[39360]	[39358]	[39360]	[39358]	[39358]	[39358]	[39358]	[39358]
	64													
4	8	35823	35833	35828	35734	35739	35737	35737	35737	35737	35737	35737	35737	35737
	16	-459	-471	-449	-415	-459	-199	-219	-208	-205	-205	-205	-69	-70
	32	35864	35862	35839	35819	35862	35862	35862	35862	35862	35862	35862	35862	35862
	64	2.1/-720	2.18/-206	2.11/-196	2.05/-99	2.11/-196	2.05/-100	2.11/-93	2.05/-83	2.05/-75	2.04/-79	2.04/-75	2.13/-10	31084
2	8	35823	35833	35828	35734	35739	35737	35737	35737	35737	35737	35737	35737	35737
	16													
	32													
	64													
1	8	37261	37277	37238	37231	37235	37235	37235	37235	37235	37235	37235	37235	37235
	16	-456	-473	-449	-405	-405	-450	-89	-126	-115	-70	-116	-8	-23
	32	36405	36406	36403	36404	36406	36406	36406	36406	36406	36406	36406	36406	36406
	64	2.11/-210	2.75/-400	2.15/-246	2.05/-58	2.15/-246	2.05/-58	2.15/-51	2.17/-41	2.17/-35	2.06/-48	2.06/-48	2.13/-1	31008
e	8	36598	36581	36578	36578	36578	36578	36578	36578	36578	36578	36578	36578	36578
	16													
	32													
	64													
		2	2	2	2	2	2	2	2	2	2	2	2	2
		*	*	*	*	*	*	*	*	*	*	*	*	*
		**	**	**	**	**	**	**	**	**	**	**	**	**
		***	***	***	***	***	***	***	***	***	***	***	***	***
		****	****	****	****	****	****	****	****	****	****	****	****	****

** - no solution
*** - overflow

TABLE VII

SOLUTIONS OF DIFFERENCE EQUATIONS FOR HHO, SECTION I-
(all values multiplied by 10^{-4})

	$v/h = \frac{1}{2}$	$v/h = \frac{1}{4}$	$v/h = \frac{1}{8}$											
$P_0(r-h)$	$C_{H0}(I)$	$C_{H0}(II)$	$C_H(I)$	$P_0(r-h)$	$P_0(r-h)$	$C_{H0}(I)$	$C_{H0}(II)$	$C_H(I)$	$P_0(r-h)$	$P_0(r-h)$	$C_{H0}(I)$	$C_{H0}(II)$	$C_H(I)$	
36166 116 36462 0.77/101 36361	36171 69 36180 0.36/177 36166	36172 60 36179 0.36/177 36166	36176 B.L.	36166 36354 0.36/66 36260	36163 -159 36354 0.36/66 36260	36160 -156 36354 0.36/66 36260	36162 -126 36354 0.36/66 36260	36161 -158 36354 0.36/66 36260	36168 -263 36195 0.51/-112 36095	36170 -262 36197 2.01/120 36098	36167 -262 36198 2.01/120 36099	36167 -262 36198 2.01/120 36099		
B.L.			B.L.											
36696 -714 36152 2.12/-105 36305 0.06/-51 [36208]	36611 -273 36310 2.12/-81 36305 0.06/-51 [36208]	36616 -180 36316 2.12/-81 36305 0.06/-51 [36208]	36690 -242 36316 2.12/-81 36305 0.06/-51 [36208]	36546 -170 36329 1.76/-68 36350 0.13/-32 [36209]	36541 -150 36321 1.76/-58 36350 0.13/-32 [36209]	36574 -152 36322 1.76/-59 36350 0.13/-32 [36209]	36535 -128 36327 1.76/-59 36350 0.13/-32 [36209]	36589 -158 36331 1.76/-59 36350 0.13/-32 [36209]	36642 -115 36337 1.76/-59 36350 0.13/-32 [36209]	36684 -179 36335 1.76/-76 36350 0.13/-32 [36209]	36708 -199 36335 2.01/-71 36350 0.13/-32 [36209]	36700 -200 36335 2.01/-71 36350 0.13/-32 [36209]	36701 -199 36335 2.01/-71 36350 0.13/-32 [36209]	36701 -200 36335 2.01/-71 36350 0.13/-32 [36209]
[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	[36209]	
35169 -257 35212 0.15/-111 35080 0.02/-55 [35955]	35370 -739 35171 0.05/-100 35071 35065 [35970]	35376 -205 35203 0.05/-100 35071 35065 [35970]	35449 -216 35203 0.05/-100 35071 35065 [35970]	32772 -86 35656 0.75/-49 35602 35602 [35955]	32773 -111 35651 0.50/-50 35602 35602 [35955]	32773 -115 35651 0.50/-50 35602 35602 [35955]	32773 -96 35651 0.50/-50 35602 35602 [35955]	32777 -118 35659 2.18/-44 35602 35602 [35955]	32777 -68 35657 2.04/-33 35602 35602 [35955]	32777 -99 35657 2.04/-33 35602 35602 [35955]	32777 -111 35657 2.04/-42 35602 35602 [35955]	32777 -120 35657 2.04/-42 35602 35602 [35955]	32777 -120 35657 2.04/-42 35602 35602 [35955]	
[35955]	[35970]	[35970]	[35970]	[35955]	[35955]	[35955]	[35955]	[35955]	[35955]	[35955]	[35955]	[35955]	[35955]	
31257 -219 31438 0.17/-93 31323 0.11/-44 31268 [31219]	31227 -208 31205 0.05/-83 31201 31201 31201 31201 [31219]	31231 -705 31223 0.05/-83 31201 31201 31201 31201 [31219]	31234 -33 31203 0.05/-25 31201 31201 31201 31201 [31219]	31203 -69 31203 0.37/-25 31201 31201 31201 31201 [31219]	31202 -69 31203 0.37/-29 31201 31201 31201 31201 [31219]	31202 -51 31203 0.37/-29 31201 31201 31201 31201 [31219]	31202 -51 31203 0.37/-29 31201 31201 31201 31201 [31219]	31204 -70 31203 0.37/-25 31201 31201 31201 31201 [31219]	31204 -13 31203 0.37/-10 31201 31201 31201 31201 [31219]	31204 -35 31203 1.37/-10 31201 31201 31201 31201 [31219]	31204 -52 31203 1.06/-17 31201 31201 31201 31201 [31219]	31204 -52 31203 1.06/-17 31201 31201 31201 31201 [31219]	31204 -52 31203 1.06/-17 31201 31201 31201 31201 [31219]	
[31219]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	[31204]	
32290 -126 32754 1.75/-52 1.71/-43 32703 1.72/-23 32580 [32557]	32411 -70 32753 0/0 32702 32702 32702 32702 [32557]	32411 -116 32753 0/0 32702 32702 32702 32702 [32557]	32410 -76 32753 0/0 32702 32702 32702 32702 [32557]	32414 -4 32753 0/0 32702 32702 32702 32702 [32557]	32414 -23 32753 0/0 32702 32702 32702 32702 [32557]	32414 -11 32753 0/0 32702 32702 32702 32702 [32557]	32414 -23 32753 0/0 32702 32702 32702 32702 [32557]	32408 1 32753 0/0 32702 32702 32702 32702 [32557]	32408 -4 32753 0/0 32702 32702 32702 32702 [32557]	32408 -10 32753 0/0 32702 32702 32702 32702 [32557]	32408 -11 32753 0/0 32702 32702 32702 32702 [32557]	32408 -10 32753 0/0 32702 32702 32702 32702 [32557]	32408 -10 32753 0/0 32702 32702 32702 32702 [32557]	
[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	[32557]	
2	2	3	3	3	3	2	2	2	2	2	2	2	2	

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THE REVIEWS

SOLUTIONS OF DIFFERENTIAL EQUATIONS FOR $\theta(x)$, OPINION IN (x, u) .

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AppendixFormulas Used for Ordvac ProgramNotations:

$u_{i,j}$ - as discussed in Section 3

$u_{i,j}^{(n)}$ - value of function for n-th iteration

Bracketed term included only for the non-linear case.

FD - BW

$$u_{i,j+1} = r(u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + u_{i,j} + [k\gamma_0 u_{i,j}], \quad 1 \leq i \leq M-1; \quad j \geq 0$$

$$\left. \begin{array}{l} u_{0,j+1} = \phi_{j+1} \\ u_{M,j+1} = \psi_{j+1} \end{array} \right\} \quad j \geq 0$$

FD - ND

$$u_{i,j+1} = r(u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + u_{i,j} + [k\epsilon^{-1/2} u_{i,j}], \quad 1 \leq i \leq M-1; \quad j \geq 0$$

$$\text{Op I} \quad u_{0,j+1} = \frac{Hhu_g + u_{1,j+1}}{1 + Hh} \quad j \geq 0$$

$$\text{Op II} \quad u_{0,j+1} = u_{1,j} + Hh(u_g - u_{0,j}) + [k\epsilon^{-1/2} u_{0,j}] \quad j \geq 0$$

 $r = \frac{1}{2}$ only

$$\text{Op III} \quad u_{0,j+1} = \frac{u_{1,j+1} + Hhu_g + \frac{1}{2r} \{ u_{0,j} + [k\epsilon^{-1/2} u_{0,j}] \}}{1 + Hh + \frac{1}{2r}} \quad j \geq 0$$

All Options:

$$u_{M,j+1} = u_{M-1,j+1}$$

CN - BV

$$u_{i,j+1}^{(0)} = u_{i,j+1} \text{ by FD method if } r \leq \frac{1}{2}$$

$$u_{i,j+1}^{(0)} = u_{i,j} \text{ if } r > \frac{1}{2}$$

$$1 \leq i \leq M-1 ; j \geq 0$$

$$u_{i,j+1}^{(n)} = (\omega-1)(\bar{u}_{i,j+1}^{(n)} - u_{i,j+1}^{(n-1)}) + \bar{u}_{i,j+1}^{(n)}$$

where:

$$\begin{aligned} \bar{u}_{i,j+1}^{(n)} = & \frac{r}{2+2r}(u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + \frac{1}{1+r}u_{i,j} \\ & + \frac{r}{2+2r}(u_{i-1,j+1}^{(n)} + u_{i+1,j+1}^{(n-1)}) \\ & + \left[\frac{1}{1+r} k \gamma \cdot \frac{(u_{i,j+1} + u_{i+1,j+1})}{2} \right] \end{aligned}$$

where:

$$u_{i-1,j+1}^{(n-1)} = u_{0,j+1}^{(n-1)} \quad i = 1 ; j \geq 0$$

$$u_{i-1,j+1}^{(n)} = u_{i-1,j+1}^{(n)} \quad 2 \leq i \leq M-1 ; j \geq 0$$

$$u_{0,j+1}^{(n)} = \emptyset_{j+1}$$

$$m \geq 0 ; j \geq 0$$

$$u_{M,j+1}^{(n)} = \gamma_{j+1}$$

CN - ND

$$u_{1,j+1}^{(0)} = u_{1,j+1} \text{ by FD method if } r \leq \frac{1}{2}$$

$$u_{1,j+1}^{(0)} = u_{1,j} \quad \text{if } r > \frac{1}{2}$$

$0 \leq i \leq M ; j \geq 0$

$$u_{j,M+j}^{(n)} = (n-1)(\bar{u}_{1,j+1}^{(n)} - u_{1,j+1}^{(n-1)}) + \bar{u}_{1,j+1}^{(n)}$$

where:

$$\begin{aligned} \bar{u}_{1,j+1}^{(n)} = & \frac{r}{2+2r}(u_{1-1,j} + u_{1+1,j} - 2u_{1,j}) + \frac{1}{1+r}u_{1,j} \\ & + \frac{r}{2+2r}(u_{1-1,j+1} + u_{1+1,j+1}^{(n-1)}) \\ & \cdot \left[\frac{1}{1+r} k \exp \left\{ - \frac{1}{\left(\frac{u_{1,j} + u_{1,j+1}^{(n-1)}}{2} \right)} \right\} \right] \end{aligned}$$

where:

$$u_{1-1,j+1}^{(n-1)} = u_{0,j+1}^{(n-1)} \quad i = 1 ; j \geq 0$$

$$u_{1-1,j+1}^{(n)} = u_{1-1,j+1}^{(n)} \quad 2 \leq i \leq M-1 ; j \geq 0$$

$$\text{Op I} \quad u_{0,j+1}^{(n)} = \frac{Hhu_k + u_{1,j+1}^{(n)}}{1 + Hh} \quad n > 0 ; j \geq 0$$

$$\text{Op II} \quad u_{0,j+1}^{(n)} = u_{1,j} + Hh(u_k - u_{0,j}) + \left[k^{\alpha} - \frac{1}{2} u_{0,j} \right] \quad n > 0 ; j \geq 0$$

 $r = \frac{1}{2}$ only

$$\text{Op III} \quad u_{0,j+1}^{(n)} = \frac{u_{1,j+1}^{(n)} + Hhu_k + \frac{1}{2r} \left\{ u_{0,j} + \left[k^{\alpha} - \frac{1}{2} u_{0,j+1}^{(n-1)} \right] \right\}}{1 + Hh + 1/2r} \quad n > 0 ; j \geq 0$$

$$\text{All Options: } u_{M,j+1}^{(n)} = u_{M-j,1}^{(n)}$$

CNN - BW

$$\begin{aligned}
 d_0 &= 0 \\
 d_1 &= \frac{r}{2+2r}(u_{0,j} + u_{2,j} - 2u_{1,j}) + \frac{1}{1+r}u_{1,j} + \frac{r}{2+2r}u_{0,j+1} + \left[\frac{1}{1+r}k\gamma e^{u_{1,j}} \right] \quad j \geq 0 \\
 d_i &= \frac{r}{2+2r}(u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + \frac{1}{1+r}u_{i,j} + \left[\frac{1}{1+r}k\gamma e^{u_{i,j}} \right] \quad 2 \leq i \leq M-2; \quad j \geq 0 \\
 d_{M-1} &= \frac{r}{2+2r}(u_{M-2,j} + u_{M,j} - 2u_{M-1,j}) + \frac{1}{1+r}u_{M-1,j} + \frac{r}{2+2r}u_{M,j+1} \\
 &\quad + \left[\frac{1}{1+r}k\gamma e^{u_{M-1,j}} \right] \quad j \geq 0 \\
 d_M &= 0
 \end{aligned}$$

$$\begin{aligned}
 b_0 &= 0 \\
 b_1 &= -\frac{r}{2+2r} \\
 b_i &= \frac{-r/2+2r}{1 + \left(\frac{r}{2+2r}\right)b_{i-1}} \quad 2 \leq i \leq M-2 \\
 b_{M-1} &= 0
 \end{aligned}$$

$$\begin{aligned}
 q_0 &= 0 \\
 q_1 &= d_1 \\
 q_i &= \frac{d_1 + \left(\frac{r}{2+2r}\right)q_{i-1}}{1 + \left(\frac{r}{2+2r}\right)b_{i-1}} \quad 2 \leq i \leq M-1
 \end{aligned}$$

$$u_{M-1,j+1} = q_{M-1}$$

$$u_{i,j+1} = q_i - b_i u_{i+1,j+1} \quad 1 \leq i \leq M-2$$

CMM - ID Op I

$$d_0 = \frac{r}{1+2r} u_{0,0}$$

$$d_i = \frac{r}{2+2r} (u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + \frac{1}{1+r} u_{i,j} + \left[\frac{1}{1+r} k_0 - \frac{1}{1+r} u_{i,j} \right] \quad 1 \leq i \leq M-1$$

$$d_M = 0$$

$$b_0 = \frac{-1}{1+2r}$$

$$b_i = \frac{-r/2+2r}{1 + \left(\frac{r}{2+2r} \right) b_{i-1}} \quad 1 \leq i \leq M-1$$

$$b_M = 0$$

$$q_0 = \frac{d_0}{1+2r}$$

$$q_i = \frac{d_i + \left(\frac{r}{2+2r} \right) q_{i-1}}{1 + \left(\frac{r}{2+2r} \right) b_{i-1}} \quad 1 \leq i \leq M-1$$

$$q_M = \frac{q_{M-1}}{1+b_{M-1}}$$

$$u_{i,j+1} = q_i$$

$$u_{i,j+1} = q_i - b_i u_{i,j+1} \quad 0 \leq i \leq M-1$$

CNN - ND Op II $r = \frac{1}{2}$ only

$$d_0 = 0$$

$$d_1 = \frac{r}{2+2r}(u_{0,j} + u_{2,j} - 2u_{1,j}) + \frac{1}{1+r}u_{1,j} + \frac{r}{2+2r}u_{0,j+1} + \left[\frac{1}{1+r}^{ke} - \frac{1}{2}u_{1,j} \right]$$

$$d_i = \frac{r}{2+2r}(u_{i,j} + u_{i+2,j} - 2u_{i+1,j}) + \frac{1}{1+r}u_{i+1,j} + \left[\frac{1}{1+r}^{ke} - \frac{1}{2}u_{i+1,j} \right] \quad 2 \leq i \leq M-1$$

$$d_M = 0$$

$$b_0 = 0$$

$$b_1 = -\frac{r}{2+2r}$$

$$b_i = \frac{-r/2+2r}{1 + \left(\frac{r}{2+2r}\right)b_{i-1}} \quad 2 \leq i \leq M-1$$

$$b_M = 0$$

$$q_0 = 0$$

$$q_1 = d_1$$

$$q_i = \frac{d_1 + \left(\frac{r}{2+2r}\right)q_{i-1}}{1 + \left(\frac{r}{2+2r}\right)b_{i-1}} \quad 2 \leq i \leq M-1$$

$$q_M = \frac{q_{M-1}}{1+b_{M-1}}$$

$$u_{M,j+1} = q_M$$

$$u_{i,j+1} = q_i - b_i u_{i+1,j+1} \quad 1 \leq i \leq M-1$$

CNN - ND Op III'

$$c_0 = \frac{Hh}{\epsilon} + \frac{1}{2r} \left\{ u_{0,j} + \left[k\epsilon^{-1/2} u_{0,j} \right] \right\}$$

$$d_1 = \frac{r}{2+2r} (u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + \frac{1}{1+r} u_{i,j} + \left[\frac{1}{1+r} k\epsilon^{-1/2} u_{i,j} \right]$$

$1 \leq i \leq M-1$

$$d_M = 0$$

$$b_0 = \frac{-1}{1+Hh+1/2r}$$

$$b_i = \frac{-r/2+2r}{1+\left(\frac{r}{2+2r}\right)b_{i-1}}$$

$1 \leq i \leq M-1$

$$b_M = 0$$

$$q_0 = \frac{d_0}{1+Hh+1/2r}$$

$$q_i = \frac{d_1 + \left(\frac{r}{2+2r}\right) q_{i-1}}{1 + \left(\frac{r}{2+2r}\right) b_{i-1}}$$

$1 \leq i \leq M-1$

$$q_M = \frac{q_{M-1}}{1+b_{M-1}}$$

$$u_{M,j+1} = q_M$$

$$u_{i,j+1} = q_i - b_i u_{i+1,j+1} \quad 0 \leq i \leq M-1$$

DEF

Compute 2^k rows by FD technique using r^i , where $r = r^i \cdot 2^k$; $0 \leq r^i \leq \frac{1}{2}$.

Let 2^k th row by $j = 1$ (first row) for DF. Then:

$$u_{i,j+1} = \frac{2r}{1+2r}(u_{i-1,j} + u_{i+1,j} - 2u_{i,j}) + u_{i,j-1} + \left[\frac{2}{1+r} - k\epsilon^i \right]$$

$1 \leq i \leq M-1; j \geq 1$

where $\epsilon^i = \begin{cases} u_{i,j} & \text{BV} \\ -1/u_{i,j} & \text{ND} \end{cases}$

The boundary conditions are the same as for the FD method, both BV and ND.

1.

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